Application of Astrium's CryoROC Code to a Single Injector Problem

A contribution to the RCM-3 Mascotte Test Case (60 bar)

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Introduction, Motivation and Objectives

This paper presents a numerical analysis of the RCM-3 Mascotte test case (60 bar) with CryoROC, Astrium's advanced multiphase Navier-Stokes solver. The CryoROC spray combustion CFD-code was developed and intended to simulate the flowfield and the heat exchange within existing and future cryogenic rocket thrust chambers. For that purpose, the computational approach so far excluded too much effort on precise modelling the vicinity of the injector head with its single elements. It's rather a question of whether the code's predictions are efficient, fast and precise enough regarding the whole thrust chamber and its global characteristics. The CryoROC code is an important tool used in the thrust chamber layout process at Astrium.

The motivation for this work thus came from two points: on one hand, it would be an interesting question, whether the code is capable to resolve the complex combustion phenomena in detail near the injector head, when the computational mesh is adequately refined in that area. One the other hand allows the workshop a further assessment of the CryoROC computation results by comparison with experimental data and other computations. This procedure is intended to analyse and to evaluate the impact of the injector-nearfield flow evolution on the overall combustion process, i.e. answering the question whether it is necessary to resolve the injector-nearfield flow phenomena *en détail* to predict global engine characteristics as the wall heat transfer accurately? Or if that is only of minor importance because there are only negligible differences a short distance further downstream the injector head, which are anyway included in the spray initialisation process?

The numerical code CryoROC

Thrust chamber flows of cryogenic hydrogen/oxygen rocket engines are characterised by the coexistence and complex interaction of various physical phases. A reactive multi-species gas mixture (1st phase), together with a dispersed oxygen droplet phase (2nd phase) have to be resolved efficiently. CryoROC treats the gaseous phase by solving the Favre-averaged Navier-Stokes equations extended by the species continuity and k-ε turbulence

Capabilities

- compressible - sub-, trans- and supersonic
- turbulence models
  - standard k - ε with wall functions
  - 2 layer model
  - compressibility effects
- multi-gaseous species consideration (H_2, O_2, H_2O, H, OH, N_2, CO_2, CO, ...etc.)
- chemical reaction models
  - turbulence controlled (Eddy Dissipation Concept)
  - kinetically controlled (Arrhenius)
  - multi-step global reaction schemes
  - * hydrogen/oxygen
- Lagrangian particle tracking (Stochastic Separated Flow model)
  - multi-class, bi-propellant, discrete particle injection and sequential tracing approach
  - mass, momentum and heat coupling with gas phase
  - supercritical LOX gasification model

Capabilities (cont.)

- viscous heating, species diffusion
- standard Jannaf property data base for gaseous combustion species (Gordon & McBride)
- porous walls and crack simulation
- coupling with Astrium's RCFS (Regenerative Coolant Flow Simulation) code

Numerics

- 2D, axisymmetric, finite volume
- Favre-averaged
- SIMPLE algorithm (pressure correction)
- implicit Stone solver

Grid

- structured
- non-orthogonal
- curvilinear

Table 1: Specification of CryoROC (***Cryo***genic ***RO***cket ***C***ombustion) Code

equations. The latter include appropriate modifications accounting for compressibility effects and handle the near wall region optionally by a logarithmic wall function approximation or by a two-layer approach. The set of equations is discretized according the finite-volume methodology for non-orthogonal, boundary fitted grids and solved by an implicit algorithm. Hereby, both central and upwind differencing schemes are applied. The reaction mechanism of cryogenic hydrogen/oxygen systems is represented by 5 species (H_2, O_2, H_2O, H and OH). Up to now, a single-step, global reaction scheme is employed (H_2 + xO2 $\Rightarrow$ aH_2O + bH + cOH) basing on a turbulence (EDC) and/or kinetically (Arrhenius) controlled combustion model.

In addition to solving transport equations for the continuous gas phase, CryoROC allows to simulate multiple discrete phases in a Lagrangian frame of reference. These second phases consist of spherical particles representing propellant droplets of different sizes being dispersed in the continuous gaseous phase. CryoROC computes the trajectories of these discrete phase entities by integrating their force balance. In particular for LH2/LOX systems, CryoROC allows for transient LOX droplet heat-up, supercritical LOX gasification, as well as droplet-to-gas phase turbulent interaction.

Gaseous and dispersed phase calculations are coupled in a loosely manner, i.e. source terms in the respective governing equations are not updated simultaneously. As a thumb rule, oxygen droplet tracking is performed every 70 to 200 gas phase iterations. Table 1 gives a survey on the most important modelling features of the CryoROC software. For a more detailed description of the models the reader is referred to [1], [2],[3].

Computational Results

Since the CryoROC code so far has only been applied to entire thrust chamber configurations, see e.g. [4], some simplistic assumptions are necessary to take, in order to receive a certain degree in reliability and efficiency. Firstly, the spray initialisation has to get adapted, because a detailed resolution of the single injector elements is not possible within that context. In particular, primary atomisation processes and 3-dimensional effects have to be excluded to enable an efficient handling. The approach chosen corresponds with concept #1 in Figure 1 and is referred as standard in the following. Here the H_2 and LOX are perfectly mixed throughout the injector element diameter so that the global mixture ratio fits exactly. Because of the finite number of injector elements inside an injector row, this approach is assumed to be rather appropriate and realistic for axisymmetric thrust chamber computations. It might not be quite as appropriate for single element calculations, as already hinted in Figure 1.

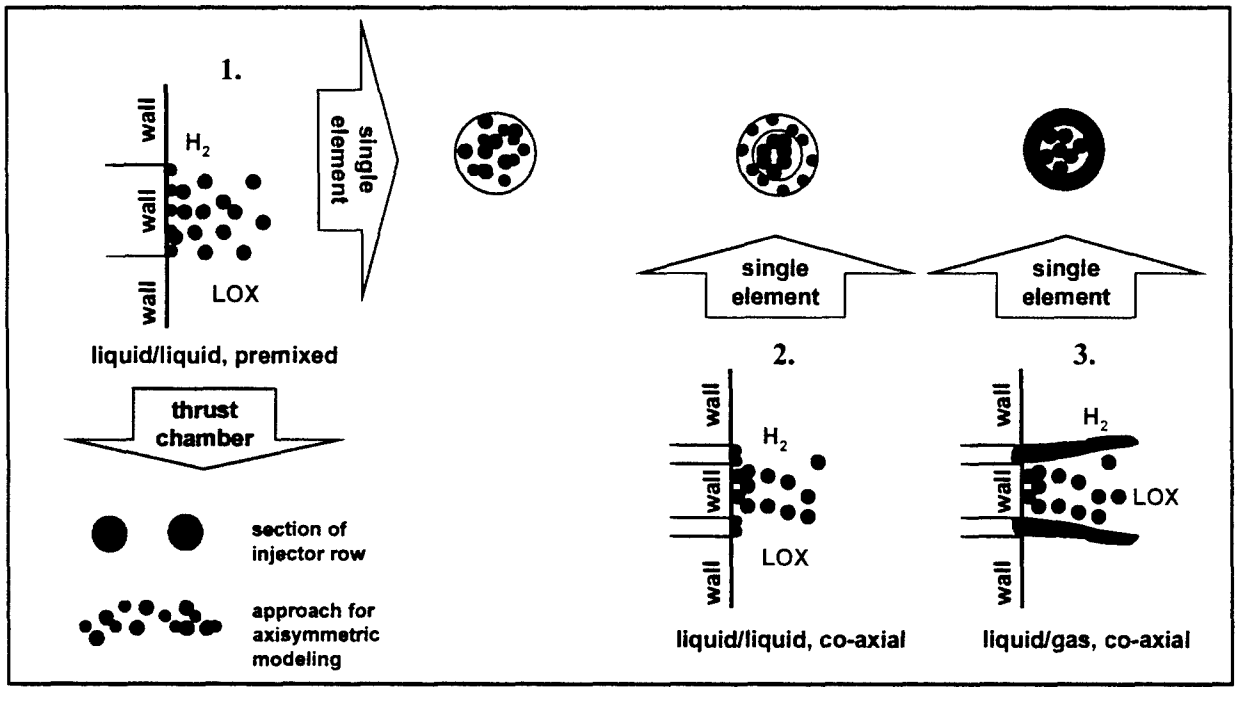


Figure 1: Spray Initialisation Concepts 1. - 3. Applied to the "Single Element Problem"

The other major assumption made for standard thrust chamber computations lies in the fact that both, oxygen as well as hydrogen, are injected in the chamber as dispersed and liquid droplets. The hydrogen, of course, is evaporated instantly. This has several advantages, but above all does that enable CryoROC to simplify the

boundary condition at the injector head. Propellant inflow is realised solely by spray initialisation, so that the wall remains closed and only an adaptation of the conservation equations' source terms is needed.

As one can recognise from Figure 1, in order to contribute to the Mascotte test case and to apply the CFD code to a single injector problem, different methods have been elaborated and applied. Apart from the standard concept #1, the concept #2 gives room to a more detailed resolution of the injector-nearfield, i.e. H_2 and LOX are now initialised co-axial but still as droplet sprays with instantaneously evaporating H_2. Concept #3 at last removes that restriction too, the way that now gaseous H_2 and dispersed O_2 are injected co-axial in accordance with the injector geometry (Figure 1). Concept #2 and #3 are assumed to be more realistic approaches to simulate axisymmetric single injectors, but less appropriate to simulate axisymmetric spray combustion within a multi-element combustor.

The Figures 2 and 3 show the computational mesh. After all, the mesh resolution still isn't fine enough to resolve the LOX post and the taper geometry and this, by the way, is assumed to be responsible for the fact that the onset of the combustion process, i.e. the anchoring of the flame front, is not captured closer to the wall in neither computation (see Figure 4).

Figure 4 reveals the temperature flowfield for all three initialisation concepts. As expected, concept #1 is not suited to resolve the flowfield phenomena in the vicinity of the injector. Best results, as far as we think to know, delivers us concept #2. Here, the flame front is clearly resolved and the flame angle coincide fairly well with that resulting from Abel-transformed emission imaging ($\approx 4°$). Moreover, the flame length seems to be realistic and compares well with what is known from experimental observations.

The alternative concept #3 looks alike, but mixture happens much sooner which leads to a much smaller combustion zone compared to concept #2. This is probably due to the specified inflow turbulence (5%), which could be too high. Reducing the incoming turbulence should lead to less diffusion and therefore to a flow field similar to concept #2. But what is more important here, is the fact that changing boundary conditions from wall to incoming mass flux condition, in order to simulate the gaseous H_2 inflow, have a dramatic effect on numerical stability and convergence behaviour. Especially the convergence criterion is only reached about a factor 10 later. Since we have to keep in mind the accessibility of the code to actual design problems with "over-night" reaction times demanded, it can be stated that this approach is far too time consuming and therefore ruled out for complex thrust chamber design applications.

As illustrated by other test case contributions, injection concept #3 is the standard for spray combustion codes. To elongate the (unrealistic) combustion zone, therefore, different correcting measures are applied. The most popular are to increase the LOX droplet injection velocities (SNECMA) or to split up the oxygen inflow into a liquid and a gaseous portion (CNES). Both measures, however, violate the inflow momentum ratio between fuel and oxidiser when a real gas approach is not taken into account. With concept #2, these boundary condition infringements could be avoided.

The OH mass fraction contours (Figure 5) give the same tendency. The development of the temperature profiles along the chamber towards the throat is shown in Figure 6. One can recognise different patterns at the start due to the different spray initialisation, which is not so much a surprise. The important point here to notice is the fact that these discrepancies will vanish after a certain distance. This becomes even more clear in Figure 7, where the (cross sectional averaged) axial temperature profiles are shown: the discrepancies exist at the start-up, but after about 0.2 m downstream, the temperature levels became very similar in all three computations. This ensures the applicability of the concept #1, i.e. it proves that one can satisfy industrial needs without resolving the flow phenomena in the injector near-field. Besides, to overcome the delayed combustion onset in concept #1, it may be suitable to reduce the O_2 - mass mean diameter and hence to adopt the spray characteristics to the assumed pre-mixed conditions.

Conclusion

The single element Mascotte test case RCM-3 has been calculated with Astrium's multi-phase Navier-Stokes code CryoROC. To take into account for thrust chamber applications' unusual single element configuration, three different propellant initialisation concepts, characterised by gaseous or dispersed hydrogen, pre-mixed or co-axial injection, have been applied and their results compared.

The concept #3 (gaseous H_2, co-axial) showed the worst convergence behaviour (about a factor 10) and is therefore ruled out for complex thrust chamber simulations. The flame could be resolved best by the concept #2 (dispersed H_2, co-axial), but as it is shown, the far-field of the injector is only slightly affected by the individual

spray initialisation concept and this outlines the applicability of concept #1 (dispersed H_2, pre-mixed) to complex thrust chamber simulations.

Note, that since there aren't any reliable experimental results available yet, a thorough assessment of the CFD results seems to be obsolete at this point.

References

[1] Knab O., Fröhlich A. and Wennerberg D.
Design Support for Advanced Storable Propellant Engines by ROCFLAM Analyses,
AIAA 99-2459, 1999.

[2] Preclik D., Estublier D. and Wennerberg D.
An Eulerian-Lagrangian Approach to Spray Combustion Modelling for Liquid Bi-Propellant Rocket Motors, AIAA 95-2779, 1995

[3] Preclik D., Wiedmann D., Oechslein W. and Kretschmer J.
Cryogenic Rocket Calorimeter Chamber Experiments and Heat Transfer Simulations,
AIAA 98-3440, 1998

[4] Wennerberg D., Knab O.
Effective Calculation of Multiphase flow Fields in Liquid Rocket Thrust Chambers,
AIAA-2001-3407, 2001

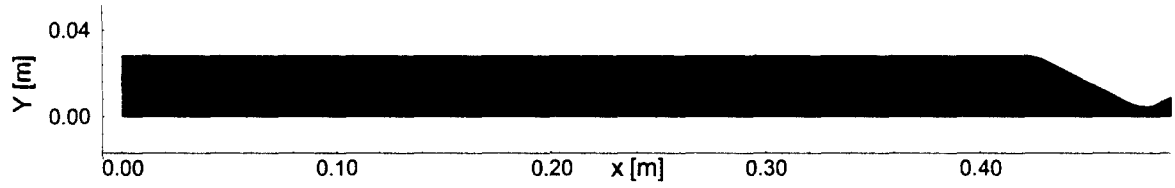


Figure 2: Computational Mesh 512x101

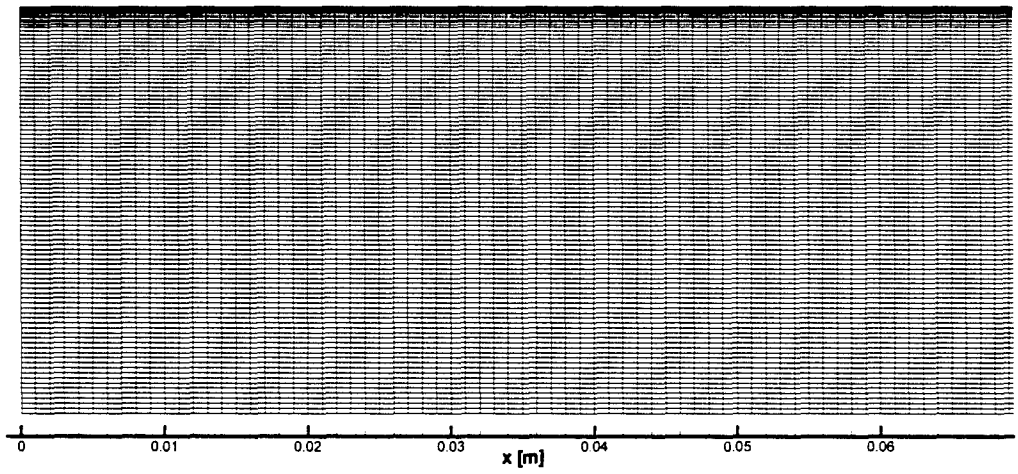


Figure 3: Zoom of the Computational Mesh, Injector Near-Field and Boundary Layer

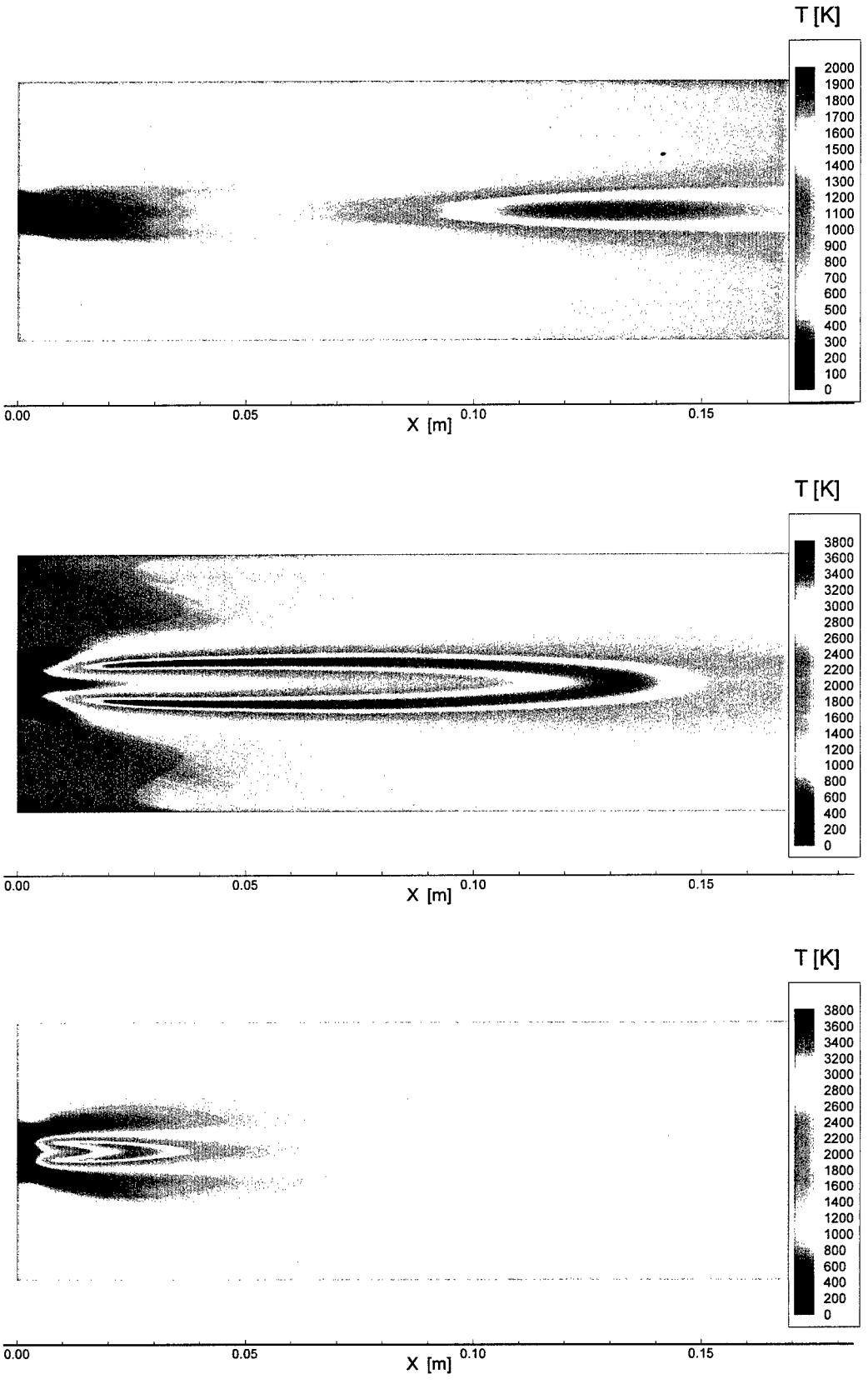


Figure 4: Temperature Contours for Spray Initialisation Concept 1 (top), 2 (middle) and 3 (bottom)

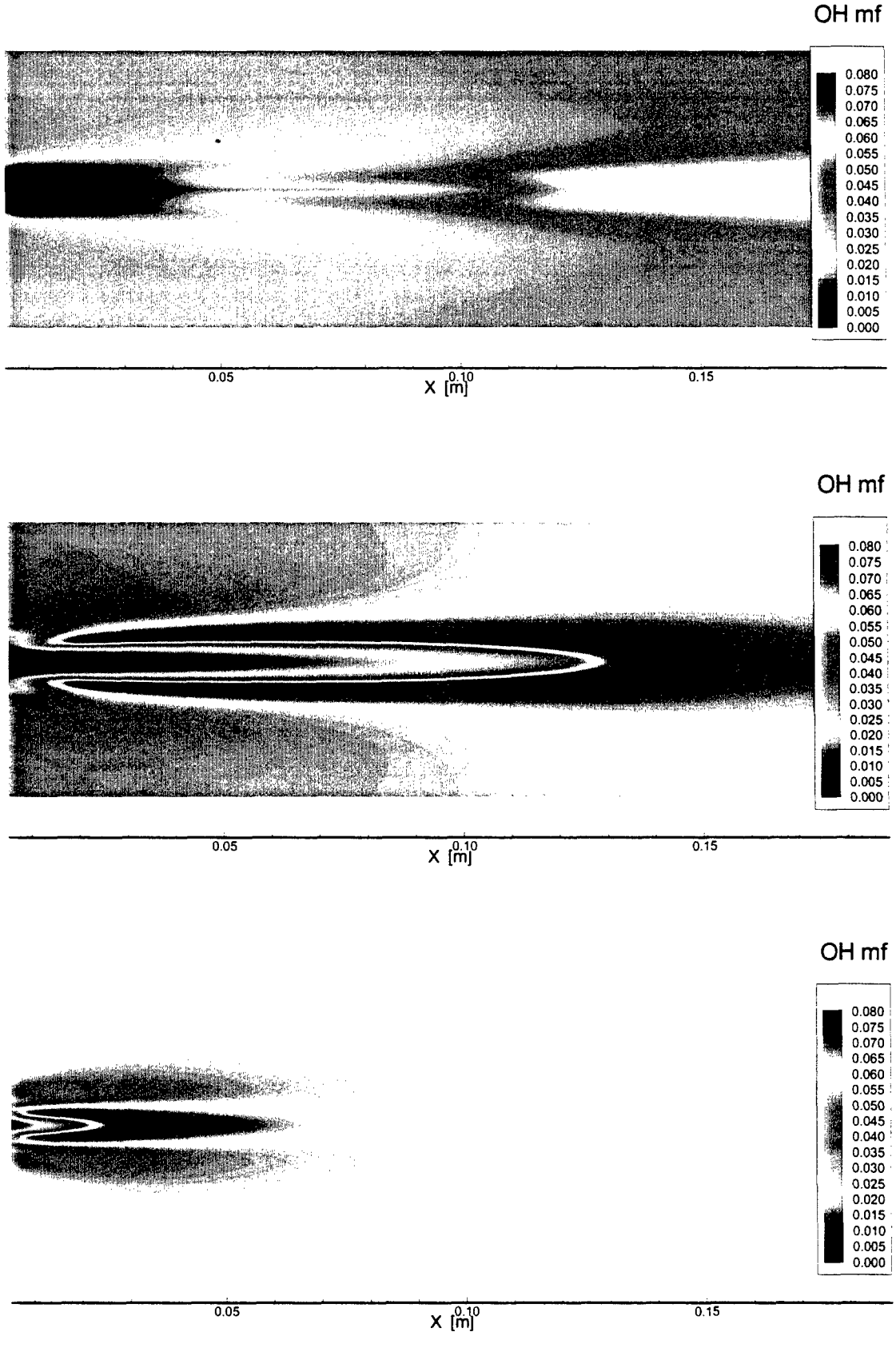
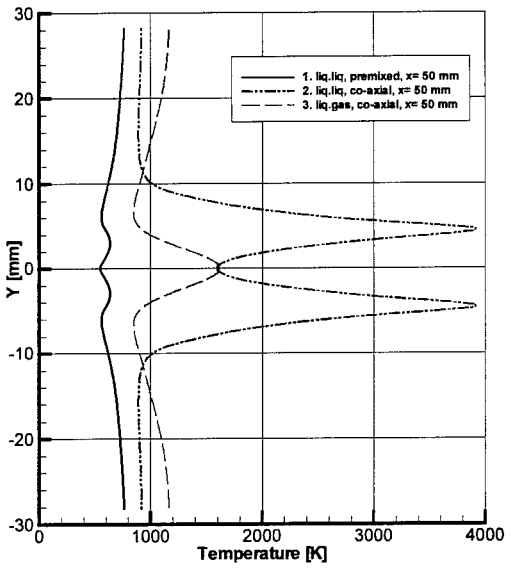


Figure 5: OH Mass Fraction Contours for Concept 1 (top), 2 (middle) and 3 (bottom)



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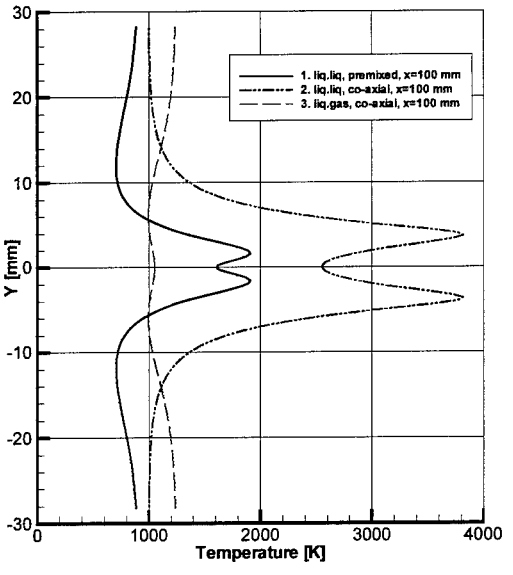

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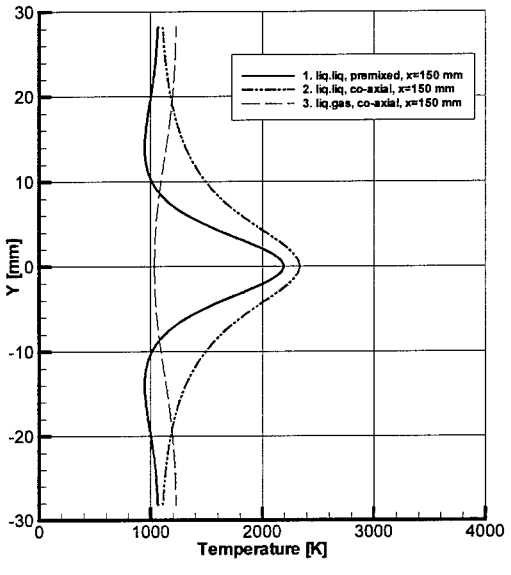

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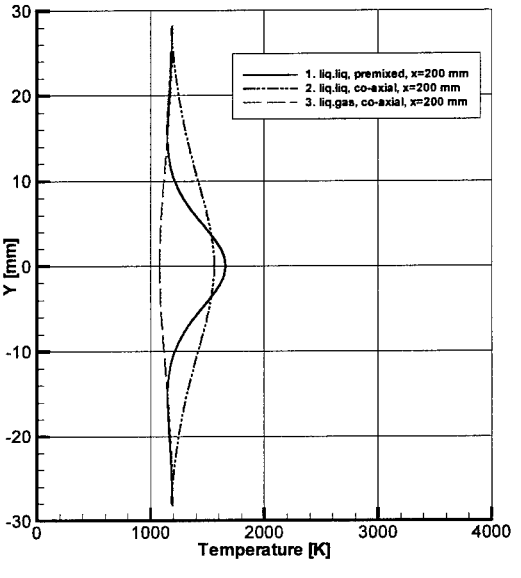

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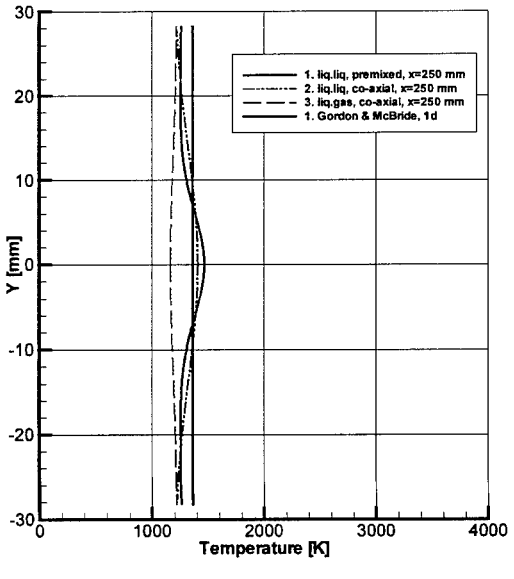

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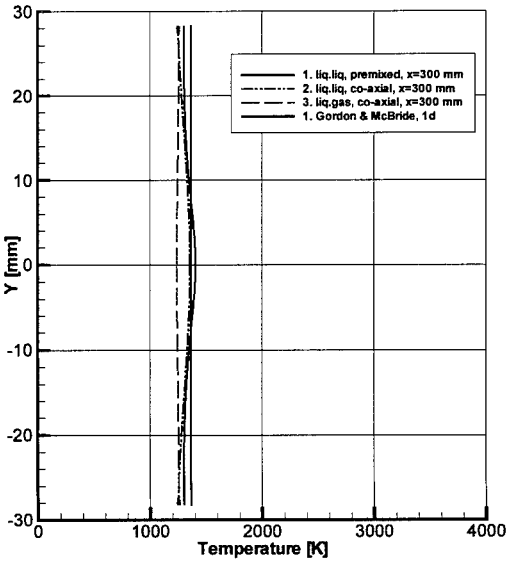

x = 300 mm

Figure 6: Temperature Profiles at Different Axial Locations

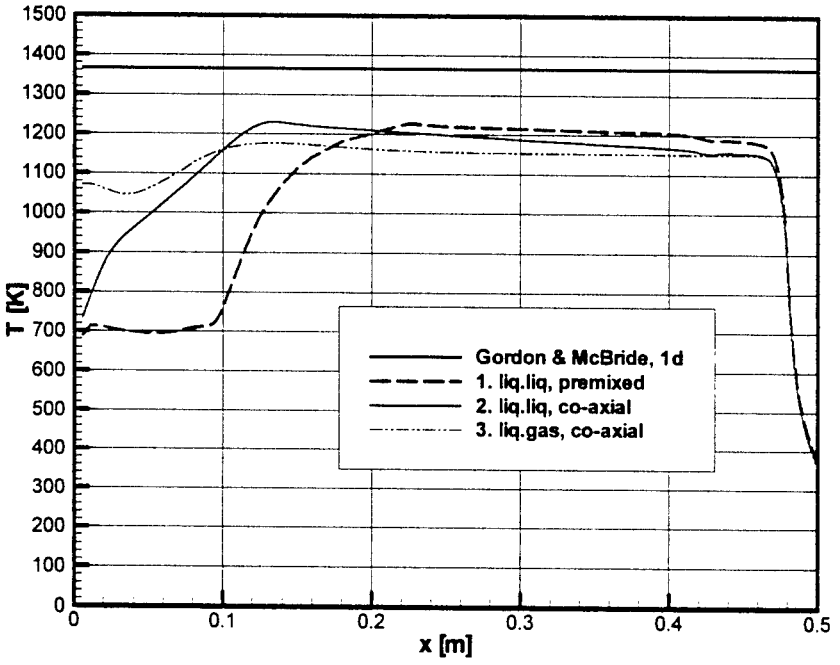

Figure 7: Cross Sectional Averaged Temperature Profiles